RESEARCH ACCOMPLISHMENTS AND PLAN

CHIN HOW JEFFREY PANG

I work on theoretical and numerical aspects of continuous optimization. My recent work has focused on variational analysis (more specifically, set-valued analysis and semi-algebraic variational analysis), differential inclusions (which is seen as a broad unifying framework for modern calculus of variations and optimal control) and numerical methods for the mountain pass problem. Variational analysis is a broad spectrum of modern mathematical theory arising from optimization, equilibrium, control and stability of linear and nonlinear systems as presented in the Lanchester prize winning work [RW98]. Other references include [AF90, BZ05, Cla83, CLSW98, DR09, Mor06].

1. Set-valued maps in the analysis of optimization problems

For a *set-valued map* $S:\mathbb{R}^n \rightrightarrows \mathbb{R}^m$ (i.e., $S(x)\subset\mathbb{R}^m$ for all $x\in\mathbb{R}^n$) and function $\varphi:\mathbb{R}^n\times\mathbb{R}^m\to\mathbb{R}$, the *marginal function* $f:\mathbb{R}^n\to\mathbb{R}$ is defined by

$$f(x) := \min_{y\in S(x)} \varphi(x,y). \tag{1}$$

It is known in the convex case that the subdifferential $\partial f(\bar{x})$ of a marginal function can be calculated using the coderivatives $D^*S(\bar{x}\mid\bar{y}):\mathbb{R}^m\rightrightarrows\mathbb{R}^n$ via

$$\partial f(\bar{x}) = \{x^* + D^*S(\bar{x}\mid\bar{y})(y^*) \mid (x^*,y^*)\in\partial\varphi(\bar{x},\bar{y})\} \text{ for any } \bar{y}\in S(\bar{x}) \text{ s.t. } \varphi(\bar{x},\bar{y}) = f(\bar{x}). \tag{2}$$

The Aubin property was first defined by Aubin [Aub84] (who first called it the pseudo Lipschitz property), and is useful in the sensitivity analysis of optimization and equilibria problems. In [Pan11b], I extended the Aubin property:

Definition 1.1. [Pan11b] (Extended Aubin property) For a positively homogeneous map $H:X\rightrightarrows Y$, we say that S is *pseudo strictly H-differentiable at* $(\bar{x},\bar{y})\in\text{Graph}(S)$ if for every $\varepsilon>0$, there is a $\delta>0$ such that

$$S(x)\cap\mathbb{B}_\delta(\bar{y}) \subset S(x') + H(x-x') + \varepsilon\|x-x'\|\mathbb{B} \text{ for all } x,x'\in\mathbb{B}_\delta(\bar{x}), \tag{3}$$

where $\mathbb{B}_r(c)$ denotes ball with radius r and center c, and $\mathbb{B}=\mathbb{B}_1(0)$.

The case where $H(x)=\kappa\|x\|\mathbb{B}$ for some $\kappa\geq 0$ reduces to the Aubin property. In [Pan11b], the connection between pseudo strict differentiability and generalized metric regularity (See [Iof00] and other texts in variational analysis) and linear openness were also discussed.

The Aubin criterion (See [DQZ06] and other papers by Aubin in the 80's) establishes the relationship between graphical derivatives and the Aubin property, and the Mordukhovich criterion [Mor93] establishes the relationship between coderivatives and the Aubin property. I generalized both criterions in [Pan11a] and identified a relationship between them. See also Figure 1. The generalized Mordukhovich criterion is particularly appealing. We say that $H:\mathbb{R}^n\rightrightarrows\mathbb{R}^m$ is a *prefan* if H is positively homogeneous, convex-compact-valued, and $H(\mathbb{B})\subset K\mathbb{B}$ for some $K<\infty$.

Theorem 1.2. [Pan11a] *(Extended Mordukhovich Criterion) For $S:\mathbb{R}^n\rightrightarrows\mathbb{R}^m$, and a prefan $H:\mathbb{R}^n\rightrightarrows\mathbb{R}^m$, S is pseudo strictly H-differentiable at $(\bar{x},\bar{y})$ if and only if $H\in\mathscr{H}(\overline{\text{co}}D^*S(\bar{x}\mid\bar{y}))$, where*

$$\mathscr{H}(D) := \{H:\mathbb{R}^n\rightrightarrows\mathbb{R}^m \mid \textit{ For all } p\neq 0 \textit{ and } u\in\mathbb{R}^m, \min_{y\in H(p)}\langle u,y\rangle \leq \min_{v\in\overline{co}D(u)}\langle v,p\rangle\}.$$

(Note that $\mathscr{H}(\overline{\text{co}}D^*S(\bar{x}\mid\bar{y})) = \mathscr{H}(D^*S(\bar{x}\mid\bar{y}))$.) Moreover, $\mathscr{H}$ has a strict reverse inclusion property, i.e.

$$\mathscr{H}(D_1) \begin{matrix}\subset\\ \subsetneq\\ =\end{matrix} \mathscr{H}(D_2) \textit{ iff } \overline{\text{co}}D_1 \begin{matrix}\supset\\ \supsetneq\\ =\end{matrix} \overline{\text{co}}D_2 \quad \textit{for all positively homogeneous } D_i:\mathbb{R}^m\rightrightarrows\mathbb{R}^n, i=1,2.$$

Theorem 1.2 tells us that the coderivatives are not only useful in the calculus of marginal functions in (2), they are also related to the pseudo strict differentiability of set-valued maps. Coderivatives are also important in formulating optimality and equilibrium conditions of other complex problems (eg., variational inequalities [FP03, KS80], MPECs [FP03, LPR96, OKZ98], multiobjective optimization [Jah04, GRTZ03], and differential inclusions in Section 2. See [Mor06, Chapters 5 and 6]). It remains to be seen what further insight Theorem 1.2 can give.

2. DIFFERENTIAL INCLUSIONS AND OPTIMAL CONTROL

For a set-valued map $F : [0,T] \times \mathbb{R}^n \rightrightarrows \mathbb{R}^n$, a function $x : [0,T] \to \mathbb{R}^n$ is said to satisfy a differential inclusion if

$$x'(t) \in F(t,x) \text{ a.e.}$$

In the case where F is single-valued, we have the familiar differential equation. The differential inclusion framework, through Filippov's theorem, is being increasingly promoted as a unifying framework for modern optimal control and the calculus of variations in the recent texts [Cla83, Mor06, Smi02, Vin00]. Other classical texts on differential inclusions include [AC84, AF90]. For $\varphi : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$, the optimization problem below is often studied;

$$\begin{array}{cl} \min_{x(\cdot)\in AC([0,T],\mathbb{R}^n)} & \varphi\big(x(0),x(T)\big) \\ \text{s.t.} & x'(t) \in F\big(t,x(t)\big) \text{ a.e.} \end{array} \tag{4}$$

Here, $AC([0,T],\mathbb{R}^n)$ stands for the set of absolutely continuous functions $x : [0,T] \to \mathbb{R}^n$. A huge part of research in optimal control and differential inclusions is on necessary conditions for optimality, starting from the classical Pontryagin Maximum Principle in the 60s. Recent work on necessary conditions in differential inclusions were obtained through the work of Clarke, Loewen, Rockafellar, Vinter, Mordukhovich, Kaskosz and Lojasiewicz, Milyutin, Smirnov, Zheng, Zhu and others. (See [Cla05] or [Mor06, Chapter 6] for a survey.)

The *reachable map* $R : X \rightrightarrows X$, which is of independent interest in optimal control, is defined by

$$R(x) = \big\{ y \mid \exists x(\cdot) \in AC([0,T],\mathbb{R}^n) \text{ s.t. } x'(t) \in F\big(t,x(t)\big) \text{ a.e.}, x(0) = x \text{ and } x(T) = y \big\}.$$

With the reachable map, we can write (4) as a marginal function $f(x) = \min_{y\in R(x)} \varphi(x,y)$.

In work currently in progress, we introduce conditions so that for $X = \mathbb{R}^n$, $\overline{\text{co}}D^*R(\bar{x} \mid \bar{y}) : \mathbb{R}^n \rightrightarrows \mathbb{R}^n$ satisfies

$$\begin{array}{rcl} \overline{\text{co}}D^*R(\bar{x} \mid \bar{y})(v) & \subset & \overline{\text{co}}\{u : \exists x(\cdot), p(\cdot) \in AC([0,T],\mathbb{R}^n) \text{ s.t.} \\ & & \quad x'(t) \in F\big(t,x(t)\big), p'(t) \in -\overline{\text{co}}D^*_x F\big(t,x(t) \mid x'(t)\big)\big(p(t)\big) \text{ a.e.}, \\ & & \quad \bar{x} = x(0), \bar{y} = x(T), u = p(0) \text{ and } v = p(T)\} \text{ for all } v \in \mathbb{R}^n. \end{array} \tag{5}$$

The proof first calculates the coderivatives of $R_N : \mathbb{R}^n \rightrightarrows \mathbb{R}^n$, the reachable map of the discretized differential inclusion problem, and then uses coderivative calculus and Theorem 1.2 to approximate $\overline{\text{co}}D^*R(x \mid y)$ from $D^*R_N(x \mid y)$. We can then estimate $\partial f(x)$ through (2). This observation allows us to study how to perturb a feasible path to optimality. The optimality condition $0 \in \partial f(x)$ implies the well known (nonsmooth) Euler Lagrange and transversality conditions.

3. NUMERICAL METHODS FOR FINDING SADDLE POINTS

We begin with the definition of a mountain pass.

Definition 3.1. (Mountain pass) Consider $a,b \in X$. Let $\Gamma(a,b)$ be the set of continuous paths $p : [0,1] \to X$ such that $p(0) = a$ and $p(1) = b$. For $f : X \to \mathbb{R}$, define an *optimal mountain pass* $\bar{p} \in \Gamma(a,b)$ to be a minimizer of

$$\inf_{p\in\Gamma(a,b)} \sup_{0\leq t\leq 1} f \circ p(t). \tag{6}$$

The point $\bar{x}$ is a *critical point* if $\nabla f(\bar{x}) = 0$, and the critical point $\bar{x}$ is a *saddle point* if it is not a local extremum. The value $f(x)$ is a *critical value* if x is a critical point. See [Jab03] for an accessible reference.

The problem of finding saddle points is of huge importance in computational chemistry and some problems in numerical partial differential equations (PDEs). Surveys in computational chemistry include [HJJ00, HS05, Sch11, Wal06], as well as the recent text [Wal03]. A software for computing saddle points in chemistry is Gaussian[1]. Tools for computing transition states[2] are also included in VASP[3]. Notable work on the applications of computing saddle points in numerical PDEs and their applications include [CM93, LM91, Fen94, ABT06, GM08, HLP06].

We recall three broad methods for computing the mountain pass. See also Figure 2.

Path-based methods. In formula (6), paths in $\Gamma(a,b)$ are discretized, and perturbed so that the maximum value of f along the path is reduced. The maximizer along the path estimates the saddle point.

Quadratic model methods. Near the saddle point $\bar{x}$, the quadratic approximation is exploited for fast convergence.

[1] http://www.gaussian.com/
[2] http://theory.cm.utexas.edu/vtsttools/neb/
[3] http://cms.mpi.univie.ac.at/vasp/vasp/vasp.html

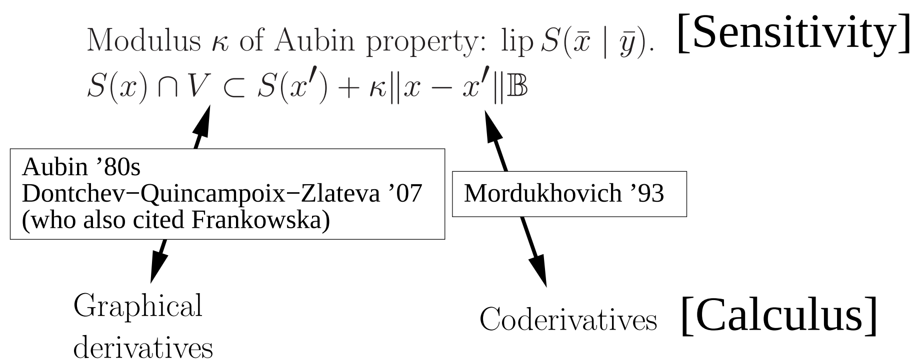

FIGURE 1. This diagram summarizes the relationship between the Aubin property, graphical derivatives (derived from tangent cones of Graph(S)) and coderivatives (derived from normal cones of Graph(S)). The graphical derivatives and coderivatives are easier to calculate and establish calculus rules, while the Aubin property is directly related to sensitivity analysis. Other than those mentioned in the figure, others who have made progress on the relation between the Aubin property and the graphical derivatives and coderivatives include Robinson, Ursescu, Rockafellar, Ioffe, Jourani, Thibault and Shao.

Level set methods. In [LP11, MF01], a different strategy involves *level sets*

$$\text{lev}_{\leq l} f := \{x : f(x) \leq l\}.$$

If l increases till components of $\text{lev}_{\leq l} f$ coalesce, then the point of coalescence is a saddle point. See Figure 2.

In ongoing work, we identify two principles desirable for a robust mountain pass algorithm:

(P1) For $f \in \mathscr{C}^2$, the algorithm has fast local convergence to a saddle point.
(P2) The global algorithm should find a saddle point of mountain pass type.

Of the above methods, path-based methods excel in (P2) but not (P1), and quadratic model methods excel in (P1) but not (P2). Through [LP11] and work in progress, we show that level set methods have midrange performance in both (P1) and (P2). Property (P2) for level set methods rely on the following property:

- For a neighborhood U and $\{l_i\}$ such that $l_i \nearrow \bar{l}$, if points x_i and y_i are in different components of $U \cap \text{lev}_{\leq l_i} f$ such that $\lim x_i = \lim y_i = \bar{x}$, then $\bar{x}$ is a saddle point.

Using $\nabla f(x_i)$ and $\nabla f(y_i)$, one can guess whether x_i and y_i are in separate components of $U \cap \text{lev}_{\leq l_i} f$. The choice of $\{l_i\}$ is harder though.

We believe a robust algorithm should include all three methods, but the right blend needs further study.

4. OTHER PAST RESEARCH

Semi-algebraic variational analysis. Semi-algebraic objects are defined formally through finitely many polynomials, and are important because they remove much of the difficulties in analysis that seldom occur in practical problems. Recent works promoting semi-algebraic variational analysis include [Lew07, Iof09, Dan09]. In [LP09], I proved that given a semi-algebraic function $f : \mathbb{R}^n \to \mathbb{R}$ and any point $x \in \mathbb{R}^n$, the robust regularization $f_\varepsilon : \mathbb{R}^n \to \mathbb{R}$ defined by $f_\varepsilon(x) := \max_{|x'-x| \leq \varepsilon} f(x')$ is locally Lipschitz at x for all small $\varepsilon > 0$. This result shows that Lipschitz methods almost always works in robust optimization. In [DP11], I proved that a semi-algebraic set-valued map has an appealing generic differentiability property, which led to work in Section 1.

Implicit multifunction theorems. In [Pan11c], I extended implicit multifunction theorems first studied in [Rob80, LZ99, DR09] in view of [Pan11b]. Such a result can describe the sensitivity analysis of the set of optimizers.

Pseudospectra. In [LP08], I studied when the pseudospectra, popularized in [TE05], is Lipschitz in the set-valued sense. This in turn has consequences to the Wilkinson distance (the distance between a matrix to the closest matrix with repeated eigenvalues), the stability of eigendecompositions in matrices, and the controllability of certain systems.

5. RESEARCH PLANS

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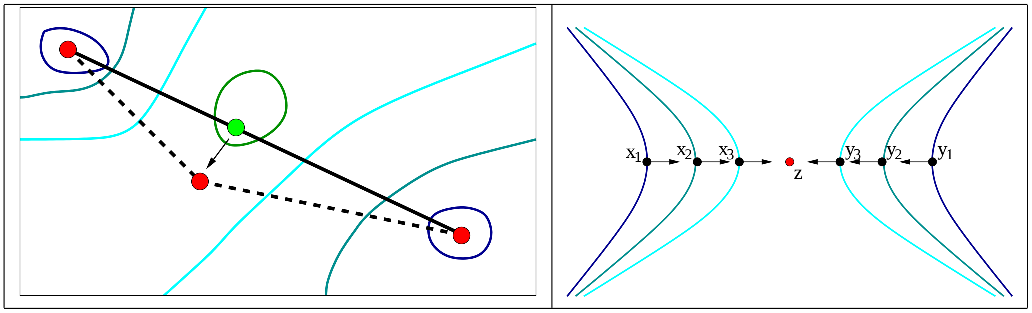

FIGURE 2. The left illustrates path-based methods, and the right illustrates level set methods

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